Exact Solution for Three-Dimensional Ising Model

Degang Zhang[1,2]

[1] *College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu 610101, China*
[2] *Institute of Solid State Physics, Sichuan Normal University, Chengdu 610101, China*

Three-dimensional Ising model in zero external field is exactly solved by operator algebras, similar to the Onsager's approach in two dimensions. The partition function of the simple cubic crystal imposed by the periodic boundary condition along both (010) and (001) directions and the screw boundary condition along the (100) direction is calculated rigorously. In the thermodynamic limit an integral replaces a sum in the formula of the partition function. When the z axis is chosen as the transfer matrix direction, a order-disorder transition in the infinite crystal occurs at a temperature $T = T_c$ determined by the condition: $\sinh \frac{2J}{k_B T_c} \sinh \frac{2(J_1+J_2)}{k_B T_c} = 1$, where $(J_1 J_2 J)$ are the interaction energies in three directions, respectively. The analytical expressions for the internal energy and the specific heat are also given. It is also shown that the thermodynamic properties of 3D Ising model with $J_1 = J_2$ are connected to those in 2D Ising model with the interaction energies $(J_1 J_{2D})$ by the relation $(\frac{J_{2D}}{k_B T})^* = (\frac{J}{k_B T})^* - \frac{J_1}{k_B T}$, where $x^* = \frac{1}{2}\ln\coth x = \tanh^{-1}(e^{-2x})$.

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I. INTRODUCTION

The exact solution for three-dimensional (3D) Ising model has been one of the greatest challenges to the physics community for decades. In 1925, Ising presented the simple statistical model in order to study the order-disorder transition in ferromagnets [1]. Subsequently the so-called Ising model has been widely applied in condensed matter physics. Unfortunately, one-dimensional Ising model has no phase transition at nonzero temperature. However, such systems could have a transition at nonzero temperature in higher dimensions [2]. In 1941, Kramers and Wannier located the critical point of two-dimensional (2D) Ising model at finite temperature by employing the dual transformation[3]. About two and a half years later Onsager solved exactly 2D Ising model by using an algebraic approach [4] and calculated the thermodynamic properties. Contrary to the continuous internal energy, the specific heat becomes infinite at the transition temperature $T = T_c$ given by the condition: $\sinh \frac{2J}{k_B T_c} \sinh \frac{2J'}{k_B T_c} = 1$, where $(J' J)$ are the interaction energies along two perpendicular directions in a plane, respectively. The partition function of 2D Ising model was also re-evaluated by a spinor analysis [5]. Up to now many 2D statistical systems have been exactly solved [6].

It is well-known that 3D Ising model has not been solved exactly yet due to its complexity. Because there is no dual transformation, the critical point of 3D Ising model cannot be fixed by such a symmetry. We also note that it is difficult to write the Hamiltonian along the third dimension of 3D Ising model with periodic boundary conditions in terms of the Onsager's operators. In addition, due to the existence of nonlocal rotation, 3D Ising model seems not to be also solved by the spinor analysis. Therefore, the key to solve 3D Ising model is to find the operator expression of the interaction along the third dimension. Here we introduce a set of operators, which is similar to that in solving 2D Ising model [4]. Under suitable boundary conditions, 3D Ising model with vanishing external field can be described by the operator algebras, and thus is solved exactly.

II. THEORY

Consider a simple cubic lattice with l layers, n rows per layer, and m sites per row. Then the Hamiltonian of 3D Ising model is $H = -\sum_{i,j,k=1}^{m,n,l}(J_1\sigma^z_{ijk}\sigma^z_{i+1kj} + J_2\sigma^z_{ijk}\sigma^z_{ij+1k} + J\sigma^z_{ijk}s^z_{ijk+1})$, where $\sigma^z_{ijk} = \pm 1$ is the spin on the site $[ijk]$. Assume that ν_k labels the spin configurations in the kth layer, we have $1 \le \nu_k \le 2^{mn}$. As a result, the energy of a spin configuration of the crystal $E_{sc} = \sum_{k=1}^{l} E_1(\nu_k) + \sum_{k=1}^{l} E_2(\nu_k) + \sum_{k=1}^{l} E(\nu_k, \nu_{k+1})$, where $E_1(\nu_k)$ and $E_2(\nu_k)$ are the energies along two perpendicular directions in the kth layer, respectively, and $E(\nu_k, \nu_{k+1})$ is the energy between two adjacent layers. Now we define $(V_1V_2)_{\nu_k\nu_k} = \sum_{\nu'_k}(V_1)_{\nu_k\nu'_k}(V_2)_{\nu'_k\nu_k} = (V_1)_{\nu_k\nu_k}(V_2)_{\nu_k\nu_k} \equiv \exp[-E_1(\nu_k)/(k_BT)] \times \exp[-E_2(\nu_k)/(k_BT)]$ and $(V_3)_{\nu_k\nu_{k+1}} \equiv \exp[-E(\nu_k, \nu_{k+1})/(k_BT)]$. Here we use the periodic boundary conditions along both (010) and (001) directions and the screw boundary condition along the (100) direction for simplicity [3] (see Fig. 1). So the spin configurations along **X** direction in a layer can be described by the spin variables $\sigma^z_1, \sigma^z_2, \cdots, \sigma^z_{mn}$. Because the probability of a spin configuration is proportional to $\exp[-E_{sc}/(k_BT)] = (V_1V_2)_{\nu_1\nu_1}(V_3)_{\nu_1\nu_2}(V_1V_2)_{\nu_2\nu_2}(V_3)_{\nu_2\nu_3}\cdots(V_1V_2)_{\nu_l\nu_l}(V_3)_{\nu_l\nu_1}$, the partition function of 3D Ising model is

$$Z = \sum_{\nu_1,\nu_2,\cdots,\nu_l}(V_1V_2)_{\nu_1\nu_1}(V_3)_{\nu_1\nu_2}\cdots(V_1V_2)_{\nu_l\nu_l}(V_3)_{\nu_l\nu_1} \equiv \mathrm{tr}(V_1V_2V_3)^l. \quad (1)$$

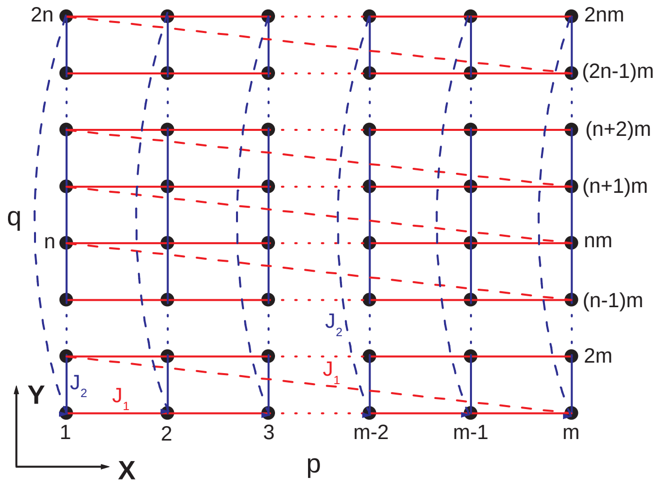

FIG. 1: (Color online) The lattice structure in each layer of the simple cubic crystal.

We note that V_1, V_2 and V_3 are 2^{mn}-dimensional matrices, and both V_1 and V_2 are diagonal. Following Ref. [4], we obtain

$$\begin{aligned} V_1 &= \exp(H_1 \textstyle\sum_{\tau=1}^{mn} \sigma_\tau^z \sigma_{\tau+1}^z) \equiv \exp(H_1 H_x), \\ V_2 &= \exp(H_2 \textstyle\sum_{\tau=1}^{mn} \sigma_\tau^z \sigma_{\tau+m}^z) \equiv \exp(H_2 H_y), \\ V_3 &= [2\sinh(2H)]^{mn/2} \exp(H^* \textstyle\sum_{\tau=1}^{mn} \sigma_\tau^x) \\ &\equiv [2\sinh(2H)]^{mn/2} \exp(H^* H_z), \end{aligned} \tag{2}$$

where $H_1 = J_1/(k_B T), H_2 = J_2/(k_B T), H = J/(k_B T)$, and $H^* = \frac{1}{2} \ln \coth H = \tanh^{-1}(e^{-2H})$.

In order to diagonalize the transfer matrix $V \equiv V_1 V_2 V_3$, following the Onsager's famous work in two dimensions, we first introduce the operators

$$L_{a,a} = -\sigma_a^x, \quad L_{a,b} = \sigma_a^z \sigma_{a+1}^x \sigma_{a+2}^x \cdots \sigma_{b-1}^x \sigma_b^z \tag{3}$$

in spin space Γ along the $\mathbf{X}$ direction under the boundary conditions mentioned above. Here $a, b = 1, 2, \cdots, 2mn$, σ_a^x, σ_a^y and σ_a^z are the Pauli matrices at site a, respectively. Then we have $L_{a,b}^2 = 1$ and

$$L_{a,b+mn} = L_{a+mn,b} = -QL_{a,b} = -L_{a,b}Q \tag{4}$$

with $Q \equiv \prod_{a=1}^{nm} \sigma_a^x = \pm 1$. It is obvious that the period of $L_{a,b}$ is 2mn. We note that these operators $L_{a,b}$ are identical to P_{ab} in Ref. [4] except mn replaces n.

H_x and H_z in the transfer matrix V can be expressed as

$$\begin{aligned} H_x &= \textstyle\sum_{a=1}^{mn} L_{a,a+1}, \\ H_z &= \textstyle\sum_{a=1}^{mn} \sigma_a^x = -\sum_{a=1}^{mn} L_{a,a}. \end{aligned} \tag{5}$$

Following Onsager's idea [4], we introduce the operators

$$\begin{aligned} \alpha_r &= -\tfrac{1}{4mn} \textstyle\sum_{a,b=1}^{2mn} L_{a,b} \cos \frac{(a-b)r\pi}{mn}, \\ \beta_r &= -\tfrac{1}{4mn} \textstyle\sum_{a,b=1}^{2mn} L_{a,b} \sin \frac{(a-b)r\pi}{mn}, \\ \gamma_r &= \tfrac{i}{8mn} \textstyle\sum_{a,b=1}^{2mn} (L_{a,x}L_{b,x} - L_{x,a}L_{x,b}) \sin \frac{(a-b)r\pi}{mn} \end{aligned} \tag{6}$$

where x is an arbitrary index. Obviously, we have $\alpha_{-r} = \alpha_r$, $\beta_{-r} = -\beta_r$, $\beta_0 = \beta_{mn} = 0$, $\gamma_{-r} = -\gamma_r$, and $\gamma_0 = \gamma_{mn} = 0$. Eqs. (6) can be rewritten as

$$\begin{aligned} \alpha_r &= -\tfrac{1}{2mn} \textstyle\sum_{s=1}^{2mn} A_s \cos \frac{rs\pi}{mn}, \\ \beta_r &= \tfrac{1}{2mn} \textstyle\sum_{s=1}^{2mn} A_s \sin \frac{rs\pi}{mn}, \\ \gamma_r &= -\tfrac{i}{2mn} \textstyle\sum_{s=1}^{2mn} G_s \sin \frac{rs\pi}{mn}, \end{aligned} \tag{7}$$

where $A_s = \sum_{a=1}^{mn} L_{a,a+s}$ and $G_s = \frac{1}{2} \sum_{a=1}^{mn} (L_{a,x}L_{a+s,x} - L_{x,a}L_{x,a+s})$. According to the orthogonal properties of the coefficients, we obtain

$$\begin{aligned} A_s &= \textstyle\sum_{r=1}^{2mn} [-\alpha_r \cos \frac{rs\pi}{mn} + \beta_r \sin \frac{rs\pi}{mn}], \\ G_s &= i \textstyle\sum_{r=1}^{2mn} \gamma_r \sin \frac{rs\pi}{mn}. \end{aligned} \tag{8}$$

From Eqs. (5)-(8), H_x and H_z have the expansions

$$\begin{aligned} H_x &= A_1 = -2 \textstyle\sum_{r=1}^{mn-1} (\alpha_r \cos \frac{r\pi}{mn} - \beta_r \sin \frac{r\pi}{mn}) \\ &\quad - \alpha_0 + \alpha_{mn}, \\ H_z &= -A_0 = \alpha_0 + 2 \textstyle\sum_{r=1}^{mn-1} \alpha_r + \alpha_{mn}. \end{aligned} \tag{9}$$

Because $A_{mn+s} = -QA_s = -A_sQ$ and $G_{mn+s} = -QG_s = -G_sQ$, and combining with Eqs. (8), we have

$$[1 + (-1)^r Q]\alpha_r = [1 + (-1)^r Q]\beta_r = [1 + (-1)^r Q]\gamma_r = 0. \tag{10}$$

When $Q = 1$, $\alpha_{2r} = \beta_{2r} = \gamma_{2r} = 0$ while $\alpha_{2r+1} = \beta_{2r+1} = \gamma_{2r+1} = 0$ if $Q = -1$. So we can investigate the algebra (8) with $Q = 1$ or -1 independently. However, we keep them together for convenience. In order to diagonalize the transfer matrix V, we must first determine the commutation relations among the operators α_r, β_r and γ_r. Similar to those calculations in Ref. [4], we obtain

$$\begin{aligned} &[A_i, A_j] = 4G_{i-j}, \quad [G_i, G_j] = 0, \\ &[G_i, A_j] = 2(A_{j+i} - A_{j-i}). \end{aligned} \tag{11}$$

Substituting Eqs. (8) into Eqs. (11), we arrive at

$$[\alpha_r, \beta_r] = 2i\gamma_r, \quad [\beta_r, \gamma_r] = 2i\alpha_r, \quad [\gamma_r, \alpha_r] = 2i\beta_r, \tag{12}$$

where $r = 1, 2, \cdots, mn - 1$, and all the other commutators vanish. Obviously, the algbra (12) is associated with the site r, and hence is local. Because α_r, β_r, and γ_r obey the same commutation relations with $-X_r$, $-Y_r$, and $-Z_r$ in Ref. [4], we have the further relations

$$\begin{aligned} &\alpha_0^2 = \tfrac{1}{2}(1 - Q) = R_0, \\ &\alpha_{mn}^2 = \tfrac{1}{2}[1 - (-1)^{mn} Q] = R_{mn}, \\ &\alpha_r \beta_r = i\gamma_r, \quad \beta_r \gamma_r = i\alpha_r, \quad \gamma_r \alpha_r = i\beta_r, \\ &\alpha_r^2 = \beta_r^2 = \gamma_r^2 = R_r^2 = R_r, \quad \alpha_r = R_r \alpha_r = \alpha_r R_r, \\ &\beta_r = R_r \beta_r = \beta_r R_r, \gamma_r = R_r \gamma_r = \gamma_r R_r. \end{aligned} \tag{13}$$

We note that $A_{sm} = \sum_{p=1}^{m} A_{p,s} = \sum_{p=1}^{m} \sum_{a=1}^{n} L_{a,a+s}^p = \sum_{p=1}^{m} \sum_{a=1}^{n} L_{p+(a-1)m,p+(a-1+s)m}$ and $G_{sm} = \sum_{p=1}^{m} G_{p,s} = \frac{1}{2} \sum_{p=1}^{m} \sum_{a=1}^{n} [L_{p+(a-1)m,x} \times$

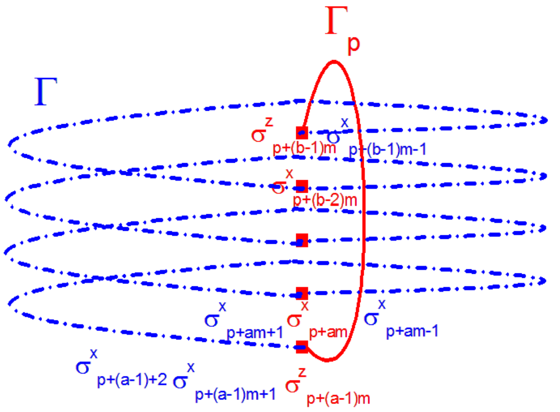

FIG. 2: (Color online) Operator renormalization: schematic of $\mathcal{L}^p_{a,b}$ in Γ_p along the $\mathbf{Y}$ direction and $L^p_{a,b}$ in Γ along the $\mathbf{X}$ direction.

$L_{p+(a-1+s)m,x} - L_{x,p+(a-1)m}L_{x,p+(a-1+s)m}]$, where $s = 1, 2, \cdots, 2n$, and

$$\begin{aligned} A_{p,s} &= \sum_{q=1}^{2n}\{-\alpha_{p+(q-1)m}\cos\tfrac{[p+(q-1)m]s\pi}{n} \\ &\quad +\beta_{p+(q-1)m}\sin\tfrac{[p+(q-1)m]s\pi}{n}\}, \\ G_{p,s} &= i\sum_{q=1}^{2n}\gamma_{p+(q-1)m}\sin\tfrac{[p+(q-1)m]s\pi}{n}. \end{aligned} \tag{14}$$

When $m = p = 1$, Eqs. (14) recover the results in two dimensions [4]. It is obvious that $A_{p,i}$ and $G_{p,j}$ also satisfy the commutation relations (11). When $p \neq p'$, $[A_{p,i}, A_{p',i'}] = [G_{p,j}, G_{p',j'}] = [A_{p,i}, G_{p',i'}] = 0$.

We have obtained the expressions of H_x and H_z in terms of the operators α_r, β_r and γ_r in the space Γ. In order to get the Hamiltonian in the third dimension, we project the operator algebra in the space Γ into the $\mathbf{Y}$ direction. Then we have m subspaces $\Gamma_p (p = 1, 2, \cdots, m)$, in which the operator algebra with period $2n$ is same with that in Γ. In Γ_p, we define

$$\begin{aligned} &\mathcal{L}^p_{a,a} = -\sigma^x_{p+(a-1)m}, \\ &\mathcal{L}^p_{a,b} = \sigma^z_{p+(a-1)m}\sigma^x_{p+am}\cdots\sigma^x_{p+(b-2)m}\sigma^z_{p+(b-1)m} \end{aligned} \tag{15}$$

along the $\mathbf{Y}$ direction. Then we have $\mathcal{A}_{p,s} = \sum_{a=1}^{n}\mathcal{L}^p_{a,a+s}$ and $\mathcal{G}_{p,s} = \frac{1}{2}\sum_{a=1}^{n}[\mathcal{L}_{p+(a-1)m,x}\mathcal{L}_{p+(a-1+s)m,x} - \mathcal{L}_{x,p+(a-1)m} \times \mathcal{L}_{x,p+(a-1+s)m}]$, which also obey the same commutation relations (11) and (12), similar to $A_{p,s}$ and $G_{p,s}$. Then the Hamiltonian $H_y = \sum_{p=1}^{m}\mathcal{A}_{p,1}$.

Because $[\mathcal{L}^p_{a,a+s}, L^p_{b,b+s}] = 0$ (see Fig. 2), we have $[\mathcal{A}_{p,s}, A_{p,s}] = 0$, which leads to $\mathcal{A}_{p,s} \equiv A_{p,s}$ due to their common local algebra (12). *This is a renormalization of operator, which means that $\mathcal{A}_{p,s}$ and $A_{p,s}$ have same eigenfunctions and eigenvalues in Γ_p or Γ space.* We note that V_2 is the transfer matrix along $\mathbf{Y}$ direction, which must be calculated in Γ rather than Γ_p space by mapping $\mathcal{A}_{p,1} \equiv A_{p,1}$ in order to diagonalize total transfer matrix V. Therefore, we have

$$\begin{aligned} H_y &= \sum_{p=1}^{m}\mathcal{A}_{p,1} = \sum_{p=1}^{m}A_{p,1} \equiv A_m \\ &= -\alpha_0 - 2\sum_{r=1}^{mn-1}(\alpha_r\cos\tfrac{r\pi}{n} - \beta_r\sin\tfrac{r\pi}{n}) \\ &\quad -(-1)^m\alpha_{mn}. \end{aligned} \tag{16}$$

Here, we would like to mention that $H_z = -\sum_{p=1}^{m}\mathcal{A}_{p,0} \equiv -A_0$, which is same with that in (9). This means that when $J_1 = 0$, the Hamiltonian of 2D Ising model is recovered immediately.

Because $[Q, H_x] = [Q, H_y] = [Q, H_z] = [Q, V] = 0$, V and Q can be simultaneously diagonalized on the same basis. In other words, the eigenvalue problem of V can be classified by the value ± 1 of Q.

The transfer matrix V with Eqs. (9) and (16) becomes

$$\begin{aligned} V &= [2\sinh(2H)]^{\frac{mn}{2}}e^{H_1A_1}e^{H_2A_m}e^{-H^*A_0} \\ &= [2\sinh(2H)]^{\frac{mn}{2}}e^{(H^*-H_1-H_2)\alpha_0} \\ &\quad \times\prod_{r=1}^{mn-1}U_re^{[H^*+H_1-(-1)^mH_2]\alpha_{mn}}, \end{aligned} \tag{17}$$

where

$$\begin{aligned} U_r &= e^{-2H_1(\alpha_r\cos\frac{r\pi}{mn}-\beta_r\sin\frac{r\pi}{mn})} \\ &\quad \times e^{-2H_2(\alpha_r\cos\frac{r\pi}{n}-\beta_r\sin\frac{r\pi}{n})}e^{2H^*\alpha_r}. \end{aligned}$$

In order to obtain the eigenvalues of the transfer matrix V, we first diagonalize U_r by employing the general unitary transformation:

$$\begin{aligned} &e^{\frac{i}{2}\eta_r\gamma_r}e^{a_r(\alpha_r\cos\theta_r+\beta_r\sin\theta_r)}U_r \\ &\times e^{-a_r(\alpha_r\cos\theta_r+\beta_r\sin\theta_r)}e^{-\frac{i}{2}\eta_r\gamma_r} = e^{\xi_r\alpha_r}. \end{aligned} \tag{18}$$

Here θ_r is an arbitrary constant and can be taken to be zero without loss of generality, and

$$\begin{aligned} &\cosh\xi_r = \mathcal{D}_r, \\ &\sinh\xi_r\cos\eta_r = \mathcal{A}_r, \quad \tanh(2a_r) = \tfrac{\mathcal{C}_r}{\mathcal{B}_r}, \\ &\sinh\xi_r\sin\eta_r = \mathcal{B}_r\cosh(2a_r) - \mathcal{C}_r\sinh(2a_r), \end{aligned} \tag{19}$$

where

$$\begin{aligned} \mathcal{A}_r &= \cosh(2H_1)\cosh(2H_2)\sinh(2H^*) \\ &\quad -\sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\cos\tfrac{r\pi}{mn} \\ &\quad -\cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\tfrac{r\pi}{n} \\ &\quad +\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{(m-1)r\pi}{mn}, \\ \mathcal{B}_r &= \sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\sin\tfrac{r\pi}{mn} \\ &\quad +\cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\sin\tfrac{r\pi}{n} \\ &\quad +\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{(m-1)r\pi}{mn}, \\ \mathcal{C}_r &= \sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\sin\tfrac{r\pi}{mn} \\ &\quad +\cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{r\pi}{n} \\ &\quad +\sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\sin\tfrac{(m-1)r\pi}{mn}, \\ \mathcal{D}_r &= \cosh(2H_1)\cosh(2H_2)\cosh(2H^*) \\ &\quad -\sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\tfrac{r\pi}{mn} \\ &\quad -\cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{r\pi}{n} \\ &\quad +\sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\tfrac{(m-1)r\pi}{mn}. \end{aligned}$$

We note that $\mathcal{D}_r^2 + \mathcal{C}_r^2 - \mathcal{A}_r^2 - \mathcal{B}_r^2 \equiv 1$, which ensures that 3D Ising model can be solved exactly in the whole

parameter space. When $H_2 = 0 (i.e. J_2 = 0)$ and $n = 1$, or $H_1 = 0 (i.e. J_1 = 0)$ and $m = 1$, we have $a_r = H^*$. So Eqs. (19) recover the Onsager's results in 2D Ising model [4].

Then the transfer matrix V has a diagonal form

$$\begin{aligned}
&e^{\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r\gamma_r}e^{\sum_{r=1}^{mn-1}a_r\alpha_r}Ve^{-\sum_{r=1}^{mn-1}a_r\alpha_r}\\
&\times e^{-\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r\gamma_r}=[2\sinh(2H^*)]^{\frac{mn}{2}}\\
&\times e^{(H^*-H_1-H_2)\alpha_0+\sum_{r=1}^{mn-1}\xi_r\alpha_r+[H^*+H_1-(-1)^m H_2]\alpha_{mn}}.
\end{aligned} \tag{20}$$

A. Transformation 1

In order to explore the symmetries in 3D Ising model, we take the transformation

$$\begin{aligned}
\alpha_r^* &= -\alpha_r\cos\tfrac{r\pi}{mn}+\beta_r\sin\tfrac{r\pi}{mn},\\
\beta_r^* &= \alpha_r\sin\tfrac{r\pi}{mn}+\beta_r\cos\tfrac{r\pi}{mn},\quad \gamma_r^*=-\gamma_r.
\end{aligned} \tag{21}$$

It is easy to prove that α_r^*, β_r^* and γ_r^* satisfy the same commutation relations with α_r, β_r and γ_r. Then we have

$$\begin{aligned}
&H_x=\alpha_0^*+2\sum_{r=1}^{mn-1}\alpha_r^*+\alpha_{mn}^*,\\
&H_y=\alpha_0^*+2\sum_{r=1}^{mn-1}[\alpha_r^*\cos\tfrac{(m-1)r\pi}{mn}+\beta_r^*\sin\tfrac{(m-1)r\pi}{mn}]\\
&\qquad-(-1)^m\alpha_{mn}^*,\\
&H_z=-\alpha_0^*-2\sum_{r=1}^{mn-1}[\alpha_r^*\cos\tfrac{r\pi}{mn}-\beta_r^*\sin\tfrac{r\pi}{mn}]+\alpha_{mn}^*.
\end{aligned} \tag{22}$$

Obviously, such a transformation exchanges the interaction forms in $(1,0,0)$ and $(0,0,1)$ directions, but changes the interaction form in $(0,1,0)$ direction. Therefore, 3D Ising model has no a dual transformation, and the critical point cannot be fixed by the Kramers and Wannier's approach [3].

The transfer matrix can be expressed as

$$\begin{aligned}
V &= [2\sinh(2H)]^{\frac{mn}{2}}e^{H_1A_1}e^{H_2A_m}e^{-H^*A_0}\\
&= [2\sinh(2H)]^{\frac{mn}{2}}e^{(H_1+H_2-H^*)\alpha_0^*}\\
&\quad\times\prod_{r=1}^{mn-1}U_r^*e^{[H_1-(-1)^mH_2+H^*]\alpha_{mn}^*},
\end{aligned} \tag{23}$$

where

$$\begin{aligned}
U_r^* &= e^{2H_1\alpha_r^*}e^{2H_2[\alpha_r^*\cos\frac{(m-1)r\pi}{mn}+\beta_r^*\sin\frac{(m-1)r\pi}{mn}]}\\
&\quad\times e^{-2H^*(\alpha_r^*\cos\frac{r\pi}{mn}-\beta_r^*\sin\frac{r\pi}{mn})}.
\end{aligned}$$

Following the procedure above, we can diagonalize the transfer matrix V, i.e.

$$\begin{aligned}
&e^{\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r^*\gamma_r^*}e^{\sum_{r=1}^{mn-1}a_r^*\alpha_r^*}Ve^{-\sum_{r=1}^{mn-1}a_r^*\alpha_r^*}\\
&\times e^{-\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r^*\gamma_r^*}=[2\sinh(2H^*)]^{\frac{mn}{2}}\\
&\times e^{(H_1+H_2-H^*)\alpha_0^*+\sum_{r=1}^{mn-1}\xi_r\alpha_r^*+[H_1-(-1)^mH_2+H^*]\alpha_{mn}^*},
\end{aligned} \tag{24}$$

where

$$\begin{aligned}
&\sinh\xi_r\cos\eta_r^*=\mathcal{A}_r^*,\quad \tanh(2a_r^*)=-\tfrac{\mathcal{C}_r}{\mathcal{B}_r^*},\\
&\sinh\xi_r\sin\eta_r^*=\mathcal{B}_r^*\cosh(2a_r^*)+\mathcal{C}_r\sinh(2a_r^*),
\end{aligned} \tag{25}$$

and

$$\begin{aligned}
\mathcal{A}_r^* &= \sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\\
&\quad-\cosh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\tfrac{r\pi}{mn}\\
&\quad-\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{r\pi}{n}\\
&\quad+\cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\tfrac{(m-1)r\pi}{mn},\\
\mathcal{B}_r^* &= \cosh(2H_1)\cosh(2H_2)\sinh(2H^*)\sin\tfrac{r\pi}{mn}\\
&\quad+\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{r\pi}{n}\\
&\quad+\cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\sin\tfrac{(m-1)r\pi}{mn}.
\end{aligned}$$

We also have $\mathcal{D}_r^2+\mathcal{C}_r^2-\mathcal{A}_r^{*2}-\mathcal{B}_r^{*2}\equiv 1$.

B. Transformation 2

Let

$$\begin{aligned}
\alpha_r' &= -\alpha_r\cos\tfrac{r\pi}{n}+\beta_r\sin\tfrac{r\pi}{n},\\
\beta_r' &= \alpha_r\sin\tfrac{r\pi}{n}+\beta_r\cos\tfrac{r\pi}{n},\quad \gamma_r'=-\gamma_r,
\end{aligned} \tag{26}$$

we have

$$\begin{aligned}
&H_x=\alpha_0'+2\sum_{r=1}^{mn-1}[\alpha_r'\cos\tfrac{(m-1)r\pi}{mn}-\beta_r'\sin\tfrac{(m-1)r\pi}{mn}]\\
&\qquad-(-1)^m\alpha_{mn}',\\
&H_y=\alpha_0'+2\sum_{r=1}^{mn-1}\alpha_r'+\alpha_{mn}',\\
&H_z=-\alpha_0'-2\sum_{r=1}^{mn-1}[\alpha_r'\cos\tfrac{r\pi}{n}-\beta_r'\sin\tfrac{r\pi}{n}]\\
&\qquad-(-1)^m\alpha_{mn}'.
\end{aligned} \tag{27}$$

The transfer matrix reads

$$\begin{aligned}
V &= [2\sinh(2H)]^{\frac{mn}{2}}e^{H_1A_1}e^{H_2A_m}e^{-H^*A_0}\\
&= [2\sinh(2H)]^{\frac{mn}{2}}e^{(H_1+H_2-H^*)\alpha_0'}\\
&\quad\times\prod_{r=1}^{mn-1}U_r'e^{[-(-1)^mH_1+H_2-(-1)^mH^*]\alpha_{mn}'},
\end{aligned} \tag{28}$$

where

$$\begin{aligned}
U_r' &= e^{2H_1[\alpha_r'\cos\frac{(m-1)r\pi}{mn}-\beta_r'\sin\frac{(m-1)r\pi}{mn}]}e^{2H_2\alpha_r'}\\
&\quad\times e^{-2H^*(\alpha_r'\cos\frac{r\pi}{n}-\beta_r'\sin\frac{r\pi}{n})}.
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
&e^{\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r'\gamma_r'}e^{\sum_{r=1}^{mn-1}a_r'\alpha_r'}Ve^{-\sum_{r=1}^{mn-1}a_r'\alpha_r'}\\
&\times e^{-\sum_{r=1}^{mn-1}\frac{i}{2}\eta_r'\gamma_r'}=[2\sinh(2H^*)]^{\frac{mn}{2}}\\
&\times e^{(H_1+H_2-H^*)\alpha_0'+\sum_{r=1}^{mn-1}\xi_r\alpha_r'+[H_2-(-1)^m(H_1+H^*)]\alpha_{mn}'}.
\end{aligned} \tag{29}$$

Here,

$$\begin{aligned}
&\sinh\xi_r\cos\eta_r'=\mathcal{A}_r',\quad \tanh(2a_r')=-\tfrac{\mathcal{C}_r}{\mathcal{B}_r'},\\
&\sinh\xi_r\sin\eta_r'=\mathcal{B}_r'\cosh(2a_r')+\mathcal{C}_r\sinh(2a_r'),
\end{aligned} \tag{30}$$

and

$$\begin{aligned}
A_r' &= \cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\\
&\quad-\cosh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\tfrac{r\pi}{n}\\
&\quad-\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{(2m-1)r\pi}{mn}\\
&\quad+\sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\cos\tfrac{(m-1)r\pi}{mn},\\
B_r' &= \cosh(2H_1)\cosh(2H_2)\sinh(2H^*)\sin\tfrac{r\pi}{n}\\
&\quad-\sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\sin\tfrac{(m-1)r\pi}{mn}\\
&\quad+\sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{(2m-1)r\pi}{mn}.
\end{aligned}$$

The identity $\mathcal{D}_r^2+\mathcal{C}_r^2-\mathcal{A}_r'^2-\mathcal{B}_r'^2\equiv 1$ also holds.

III. RESULTS

Because $\alpha_0, \alpha_1, \cdots, \alpha_{mn}$ have the common eigenvectors χ_0 with the corresponding eigenvalues $\Delta_0, \Delta_1, \cdots, \Delta_{mn}$, from Eq. (20), we have $V\psi = \lambda\psi$, where

$$\begin{aligned} \psi &= e^{-\sum_{r=1}^{mn-1} a_r \alpha_r} e^{-\sum_{r=1}^{mn-1} \frac{i}{2}\eta_r \gamma_r} \chi_0, \\ \ln\lambda &= \tfrac{1}{2} mn \ln[2\sinh(2H)] + (H^* - H_1 - H_2)\Delta_0 \\ &\quad + \textstyle\sum_{r=1}^{mn-1} \xi_r \Delta_r + [H_1 - (-1)^m H_2 + H^*]\Delta_{mn}. \end{aligned} \tag{31}$$

At the critical point, we have $\xi_0 = H^* - H_1 - H_2 = 0$ [4]. This leads to a critical temperature $T = T_c$ given by the condition

$$\sinh(2H)\sinh(2H_1 + 2H_2) = 1. \tag{32}$$

If $H_2 = 0$ or $H_1 = 0$, we obtain the critical temperature in 2D Ising model [3, 4]. We note that when $H_1 = H_2 = H$, the critical value $H_c = J/(k_B T_c) = 0.30468893$, which is larger than the conjectured value about 0.22 from the previous numerical simulations.

We note that the thermodynamic properties of a large crystal are determined by the largest eigenvalue $\lambda_{\max}$ of the transfer matrix V. Following Ref. [4], we have

$$\begin{aligned} &\ln\lambda_{\max} - \tfrac{1}{2} mn \ln[2\sinh(2H)] \\ &= \begin{cases} \xi_1 + \xi_3 + \cdots + \xi_{2L-1} & \text{for } mn = 2L; \\ \xi_1 + \xi_3 + \cdots + \xi_{2L-1} \\ \quad + H_1 - (-1)^m H_2 + H^* & \text{for } mn = 2L+1. \end{cases} \end{aligned} \tag{33}$$

Here $\Delta_1 = \Delta_3 = \cdots = \Delta_{mn-1} = 1$, which are same with the eigenvalues of the operators X_r in Ref. [4]. We note that these two results above can be combined due to $\xi_{-r} = \xi_r$ and $\xi_{mn} = 2[H_1 - (-1)^m H_2 + H^*]$. So Eqs. (33) have the compact form

$$\begin{aligned} &\ln\lambda_{\max} - \tfrac{1}{2} mn \ln[2\sinh(2H)] = \tfrac{1}{2}\textstyle\sum_{r=1}^{mn} \xi_{2r-1} \\ &= \tfrac{1}{2}\textstyle\sum_{r=1}^{mn} \cosh^{-1}[\cosh(2H_1)\cosh(2H_2)\cosh(2H^*) \\ &\quad - \sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\frac{(2r-1)\pi}{2mn} \\ &\quad - \cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\frac{(2r-1)\pi}{2n} \\ &\quad + \sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\frac{(m-1)(2r-1)\pi}{2mn}]. \end{aligned} \tag{34}$$

In order to calculate the partition function per atom $\lambda_\infty = \lim_{m,n\to\infty}(\lambda_{\max})^{\frac{1}{mn}}$ for the infinite crystal, we replace the sum in Eq. (34) by the integral

$$\ln\lambda_\infty = \frac{1}{2}\ln[2\sinh(2H)] + \frac{1}{2\pi}\lim_{m\to\infty}\int_0^\pi \xi_m(\omega)d\omega, \tag{35}$$

where

$$\begin{aligned} \cosh\xi_m(\omega) &= \mathcal{D}(\omega) = \cosh(2H_1)\cosh(2H_2)\cosh(2H^*) \\ &\quad - \sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\omega \\ &\quad - \cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos(m\omega) \\ &\quad + \sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos[(m-1)\omega]. \end{aligned} \tag{36}$$

Similarly, the continuous $\mathcal{A}(\omega)$, $\mathcal{A}^*(\omega)$, $\mathcal{A}'(\omega)$, $\mathcal{B}(\omega)$, $\mathcal{B}^*(\omega)$, $\mathcal{B}'(\omega)$, $\mathcal{C}(\omega)$, $\xi_m(\omega)$, $\eta(\omega)$, $\eta^*(\omega)$, and $\eta'(\omega)$ replace the discrete $\mathcal{A}_r$, $\mathcal{A}_r^*$, $\mathcal{A}_r'$, $\mathcal{B}_r$, $\mathcal{B}_r^*$, $\mathcal{B}_r'$, $\mathcal{C}_r$, ξ_r, η_r, η_r^*, and η_r', respectively, by letting $\omega = \frac{r\pi}{mn}$. Here we emphasis that when $H_2 = 0$, or $H_1 = 0$, Eq. (35) is nothing but the Onsager's famous result in the 2D case [4]. We also note that very different from the 2D case, the partition function of 3D Ising model is oscillatory with the system size m. Therefore, the conjectured values extrapolating to the infinite system seem to be unreliable.

For a crystal of $N = mnl$, the free energy

$$F = U - TS = -Nk_BT\ln\lambda_\infty, \tag{37}$$

the internal energy

$$\begin{aligned} U &= F - T\frac{dF}{dT} = Nk_BT^2\frac{\ln\lambda_\infty}{dT} \\ &= -Nk_BT[H_1\frac{\partial\ln\lambda_\infty}{\partial H_1} + H_2\frac{\partial\ln\lambda_\infty}{\partial H_2} + H\frac{\partial\ln\lambda_\infty}{\partial H}], \end{aligned} \tag{38}$$

and the specific heat

$$\begin{aligned} C &= \frac{dU}{dT} = Nk_B[H_1^2\frac{\partial^2\ln\lambda_\infty}{\partial H_1^2} + H_2^2\frac{\partial^2\ln\lambda_\infty}{\partial H_2^2} + H^2\frac{\partial^2\ln\lambda_\infty}{\partial H^2} \\ &\quad + 2H_1H_2\frac{\partial^2\ln\lambda_\infty}{\partial H_1\partial H_2} + 2H_1H\frac{\partial^2\ln\lambda_\infty}{\partial H_1\partial H} + 2H_2H\frac{\partial^2\ln\lambda_\infty}{\partial H_2\partial H}]. \end{aligned} \tag{39}$$

Here,

$$\begin{aligned} \frac{\partial\ln\lambda_\infty}{\partial H_1} &= \frac{1}{\pi}\lim_{m\to\infty}\int_0^\pi \cos\eta^* d\omega, \\ \frac{\partial\ln\lambda_\infty}{\partial H_2} &= \frac{1}{\pi}\lim_{m\to\infty}\int_0^\pi \frac{\frac{\partial\mathcal{D}}{\partial H_2}}{\sinh\xi_m} d\omega, \\ \frac{\partial\ln\lambda_\infty}{\partial H} &= \cosh(2H^*) - \frac{1}{\pi}\sinh(2H^*)\lim_{m\to\infty}\int_0^\pi \cos\eta d\omega, \\ \frac{\partial^2\ln\lambda_\infty}{\partial H_1^2} &= \frac{2}{\pi}\lim_{m\to\infty}\int_0^\pi \sin^2\eta^*\coth\xi_m d\omega, \\ \frac{\partial^2\ln\lambda_\infty}{\partial H_2^2} &= \frac{1}{2\pi}\lim_{m\to\infty}\int_0^\pi [4 - \frac{1}{\sinh^2\xi_m}(\frac{\partial\mathcal{D}}{H_2})^2]\coth\xi_m d\omega, \\ \frac{\partial^2\ln\lambda_\infty}{\partial H^2} &= 2\sinh^2(2H^*)[\frac{1}{\pi}\coth(2H^*)\lim_{m\to\infty}\int_0^\pi \cos\eta d\omega \\ &\quad + \frac{1}{\pi}\lim_{m\to\infty}\int_0^\pi \sin^2\eta\coth\xi_m d\omega - 1], \\ \frac{\partial^2\ln\lambda_\infty}{\partial H_1\partial H_2} &= \frac{1}{\pi}\lim_{m\to\infty}\int_0^\pi \frac{d\omega}{\sinh\xi_m}(\frac{\partial\mathcal{A}^*}{\partial H_2} - \frac{\partial\mathcal{D}}{\partial H_2}\cos\eta^*\coth\xi_m), \\ \frac{\partial^2\ln\lambda_\infty}{\partial H_1\partial H} &= -\frac{1}{\pi}\sinh(2H^*) \\ &\quad \times \lim_{m\to\infty}\int_0^\pi \frac{d\omega}{\sinh\xi_m}(\frac{\partial\mathcal{A}^*}{\partial H^*} - 2\cosh\xi_m\cos\eta\cos\eta^*), \\ \frac{\partial^2\ln\lambda_\infty}{\partial H_2\partial H} &= -\frac{1}{\pi}\sinh(2H^*) \\ &\quad \times \lim_{m\to\infty}\int_0^\pi \frac{d\omega}{\sinh\xi_m}(\frac{\partial\mathcal{A}}{\partial H_2} - \frac{\partial\mathcal{D}}{\partial H_2}\cos\eta\coth\xi_m). \end{aligned}$$

We note that at the critical point, $\lim_{\omega\to 0}\xi_m \to 0$. However, $\lim_{\omega\to 0}\frac{\partial\mathcal{D}}{\partial H_2}/\sinh\xi_m \to -\cos\eta(0)$. Therefore, we can see from Eqs. (37) and (38) that at the critical point, the internal energy U is continuous while the specific heat C becomes infinite, similar to the 2D case.

We consider the special case of $J_1 = J_2$, where the calculation of the thermodynamic functions can be simplified considerably. After integrating, Eq. (36) can be rewritten as

$$\begin{aligned} \cosh\xi_\infty(\omega) &= \cosh(2H_1)\cosh(2H_{2D}^*) \\ &\quad - \sinh(2H_1)\sinh(2H_{2D}^*)\cos\omega, \end{aligned} \tag{40}$$

where

$$H_{2D}^* = H^* - H_1. \tag{41}$$

It is surprising that Eq. (40) is nothing but that in 2D Ising model with the interaction energies (J_1, J_{2D}) and $H_{2D} = \frac{J_{2D}}{k_B T}$. Therefore, $\ln\lambda_\infty - \frac{1}{2}\ln[2\sinh(2H)]$ in three dimensions can be obtained from $\ln\lambda_\infty^{2D} - \frac{1}{2}\ln[2\sinh(2H_{2D})]$ in two dimensions by taking the transformation (41). In other words, the thermodynamic properties of 3D Ising model originate from those in 2D case. We can also see from Eq. (41) that both 2D and 3D Ising systems approach simultaneously the critical point, i.e. $H_{2D}^* = H_1$ and $H^* = 2H_1$. It is expected that the scaling laws near the critical point in two dimensions also hold in three dimensions [6].

The energy U and the specific heat C of 2D Ising model with the quadratic symmetry (i.e. $H_1 = H_{2D}$) have been calculated analytically by Onsager and can be expressed in terms of the complete elliptic integrals [4]. The critical exponent associated with the specific heat $\alpha_{2D} = 0$. Because 3D Ising model with the simple cubic symmetry (i.e. $H_1 = H_2 = H$) can be mapped exactly into 2D one by Eq. (41), the expressions of U and C in three dimensions have similar forms with those in two dimensions. So the critical exponent α_{3D} of the 3D Ising model is identical to α_{2D}, i.e. $\alpha_{3D} = 0$. According to the scaling laws $d\nu = 2-\alpha$ and $\mu+\nu = 2-\alpha$ [6], we have $\nu_{3D} = \frac{2}{3}$ and $\mu_{3D} = \frac{4}{3}$.

Up to now, we have obtained the partition function per site and some physical quantities when the z axis is chosen as the transfer matrix direction. However, if the $x(y)$ axis is parallel to the transfer matrix direction, the corresponding partition function per site can be achieved from Eqs. (35) and (36) by exchanging the interaction constants along the $x(y)$ and z axes. Therefore, the total physical quantity in 3D Ising model, such as the free energy, the internal energy, the specific heat, and etc., can be calculated by taking the average over three directions. We note that the average of a physical quantity naturally holds for 2D Ising model.

IV. HIGH TEMPERATURE EXPANSIONS

Now we calculate the high temperature expansions of the partition function per atom when $J_1 = J_2 = J$. According to the identity

$$\int_0^{2\pi} \ln(2\mathrm{cosh}x - 2\mathrm{cos}\omega')d\omega' = 2\pi x, \qquad (42)$$

from Eqs. (35) and (36), we obtain

$$\begin{aligned}
\ln\frac{\lambda_\infty}{2} &= \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln\{\mathrm{cosh}^3(2H) \\
&\quad -\mathrm{sinh}(2H)\mathrm{cosh}(2H)[\mathrm{cos}\omega + \mathrm{cos}(m\omega)] \\
&\quad +\mathrm{sinh}^2(2H)\mathrm{cosh}(2H)\mathrm{cos}[(m-1)\omega] \\
&\quad -\mathrm{sinh}(2H)\mathrm{cos}\omega'\}d\omega d\omega' \\
&= 3\mathrm{lncosh}H + \frac{3}{2}\mathrm{ln}(1+k^2) \\
&\quad +\frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln\{1 - \frac{2k(1-k^2)}{(1+k^2)^2}[\mathrm{cos}\omega + \mathrm{cos}(m\omega)] \\
&\quad +\frac{4k^2}{(1+k^2)^2}\mathrm{cos}[(m-1)\omega] \\
&\quad -\frac{2k(1-k^2)^2}{(1+k^2)^3}\mathrm{cos}\omega'\}d\omega d\omega' \\
&= 3\mathrm{lncosh}H - 3k^4 - 62k^6 - \frac{2081}{2}k^8 \\
&\quad -21024k^{10} - \cdots,
\end{aligned} \qquad (43)$$

where $k = \tanh H$. Therefore, the partition function per atom in high temperatures is

$$\lambda_\infty = 2\cosh^3 H(1-3k^4-62k^6-1036k^8-20838k^{10}-\cdots). \qquad (44)$$

We note that for periodic boundary conditions, the high temperature partition function per atom reads [7]

$$\lambda_\infty^p = 2\cosh^3 H(1+3k^4+22k^6+192k^8+2046k^{10}+\cdots). \qquad (45)$$

Obviously, the difference between λ_∞ and λ_∞^p comes from the screw boundary condition along the **X** direction (see Fig. 1).

V. CONCLUSIONS

We have exactly solved 3D Ising model by an algebraic approach. The critical temperature $T_{ic}(i = 1,2,3)$, at which an order transition occurs, is determined. At T_{ic}, the internal energy is continuous while the specific heat diverges. Obviously, the thermodynamic properties in three dimensions are highly correlated to those of 2D Ising system. When the interaction energy in the third dimension vanishes, the Onsager's exact solution of 2D Ising model is recovered immediately. This guarantees the correctness of the exact solution of 3D Ising model.

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